

Performance Assessment of a Generic Repository for Defense-Related HLW/SNF in Fractured Crystalline Host Rock – 17059

S. David Sevougian*, Emily R. Stein*, Michael B. Gross*, Glenn E. Hammond*, Jennifer M. Frederick*, and Paul E. Mariner*

*Sandia National Laboratories, PO Box 5800, MS 0747, Albuquerque, NM 87185, sdsevou@sandia.gov

ABSTRACT

Recently the U.S. made a policy decision to begin R&D for geologic disposal of defense-related HLW/SNF in a facility separate from commercially generated waste. A deep geologic repository for the disposal of DOE-managed HLW, and some thermally cooler DOE-managed SNF, arising from defense and DOE R&D activities, is part of a stepwise, phased approach for disposal of the Nation's nuclear waste, as recommended by the Blue Ribbon Commission on America's Nuclear Future. The work discussed here focuses on post-closure safety (or performance) assessment for such a Defense Waste Repository (DWR), which is divided into four major activities: (1) development of generic reference cases (i.e., knowledge or technical bases for "generic" or "non-site-specific" deep geologic repositories); (2) features, events, and processes (FEPs) analyses and screening to support the technical bases and the performance assessment (PA) model; (3) performance evaluation of alternative EBS design concepts; and (4) post-closure safety analyses of the repository system under consideration.

Using the known inventory of defense-related SNF, as well as defense-related HLW stored at the Savannah River and Hanford sites, the *Geologic Disposal Safety Assessment (GDSA) Framework* modeling and software system has been applied to simulate the potential performance of a DWR in crystalline host rock, resulting in a suite of single-realization (i.e., deterministic) and multi-realization (i.e., probabilistic) 3-D post-closure system analyses, over a performance period of one million years. Two types of emplacement concepts are examined, including single-canister vertical-borehole emplacement for the hotter defense SNF waste (KBS-3V concept) and multi-canister horizontal emplacement for defense HLW (similar to Yucca Mountain co-disposal waste packages). Sensitivity analyses examine the effect of key uncertain parameters on repository performance, including the effects of fracture distribution, waste package degradation rate, buffer and disturbed rock zone (DRZ) properties, and sorption parameters. Initial results indicate that a crystalline host rock with a connected fracture system may require additional safety features to ensure robustness of the isolation safety function, such as a deep unsaturated zone, a sufficiently thick sedimentary overburden, and/or a disposal overpack with a very slow corrosion rate. None of these should pose an undue obstacle for successful disposal.

INTRODUCTION

In October 2014, the U.S. DOE issued a report [1] describing the potential advantages for "disposal of DOE-managed HLW from defense activities and some thermally cooler DOE-managed SNF, potentially including cooler naval SNF, separately from disposal of commercial SNF and HLW." In March 2015, the U.S. President directed that such a separate repository, hereafter called a Defense Waste Repository (DWR), is required for "defense HLW" (or HLW resulting from atomic energy defense activities), based on Section 8(b)(2) of the Nuclear Waste Policy Act of 1982 and the analysis in [2]. As described in DOE (2014): "Disposal of this HLW and SNF poses the fewest challenges, potentially allowing for a simpler repository design and licensing process, while helping meet DOE's environmental management goals and building confidence in waste management practices." A recent study by the U.S. Government Accountability Office [3] has questioned some of the assumptions underlying this decision but the work described here is independent of any final societal decision on the path forward for waste disposal.

Fig. 1 shows the major components of a Safety Case for establishing confidence in the technical feasibility, safety, and performance of any deep geologic repository. Such a safety case evolves during the decades-long siting and development process of a repository project, illustrated schematically in Fig. 2. At each major milestone or stage in such a project, i.e., each Critical Decision (CD) point [4, 5] shown in Fig. 2, the primary components of the project and its safety case are updated based on the most recent information available. With respect to satisfying health and environmental safety regulations for the long-term (post-closure) performance of the disposal system, this periodic project update primarily involves the interplay between Components 3.3 and 4.2 of the Safety Case shown in Fig. 1, i.e., the evolving knowledge/engineering bases and the latest safety assessment analyses. This interplay is shown in Fig. 3, in a relational or “flow-diagram/information-feed” fashion. The U.S. repository program for defense, as well as commercial, nuclear waste is currently at the indicated location on the timeline in Fig. 2, corresponding to *generic* (“non site-specific”) R&D only. At this early stage, no specific dates for future CD points have been scheduled.

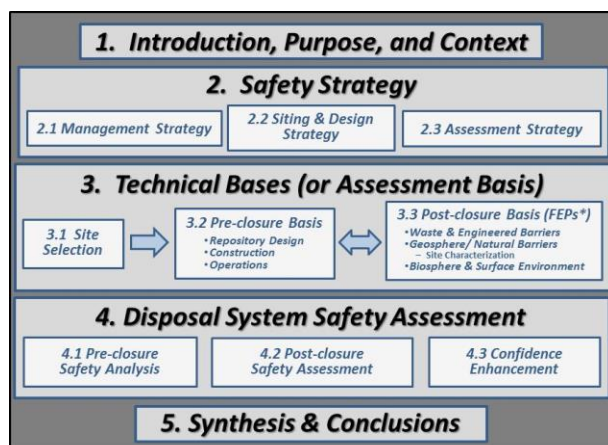


Fig. 1. Major components of the Safety Case [6].

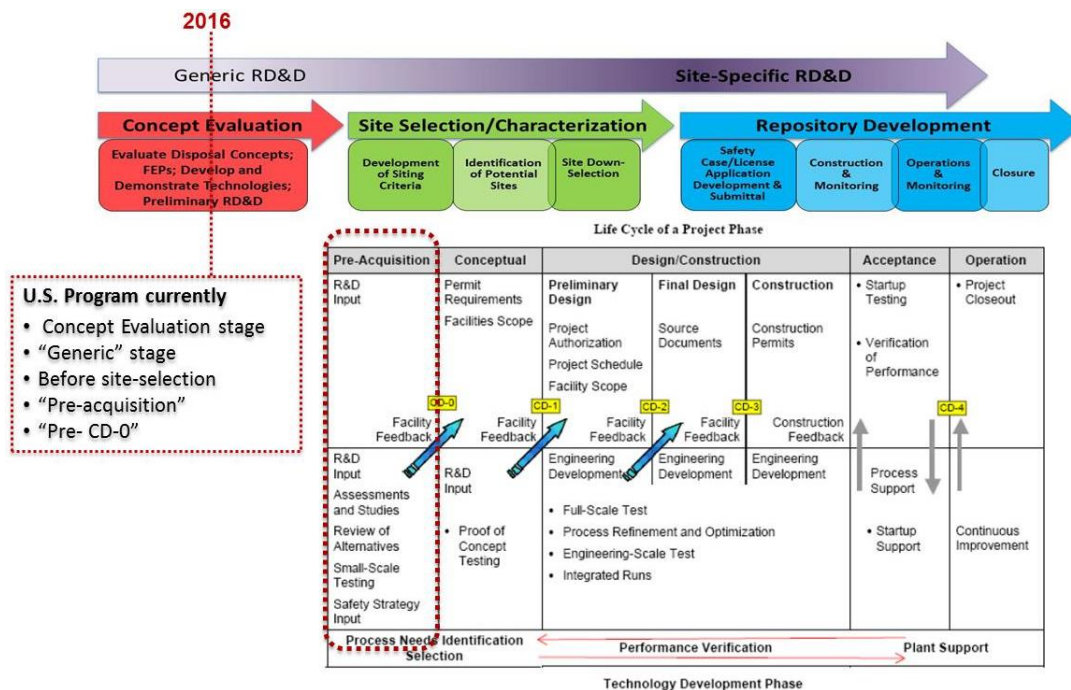


Fig. 2. Illustrative timeline for a repository project and associated R&D [7]. {"Life Cycle of a Project Phase" illustrates the key Critical Decision (CD) points described in [4] and [5].}

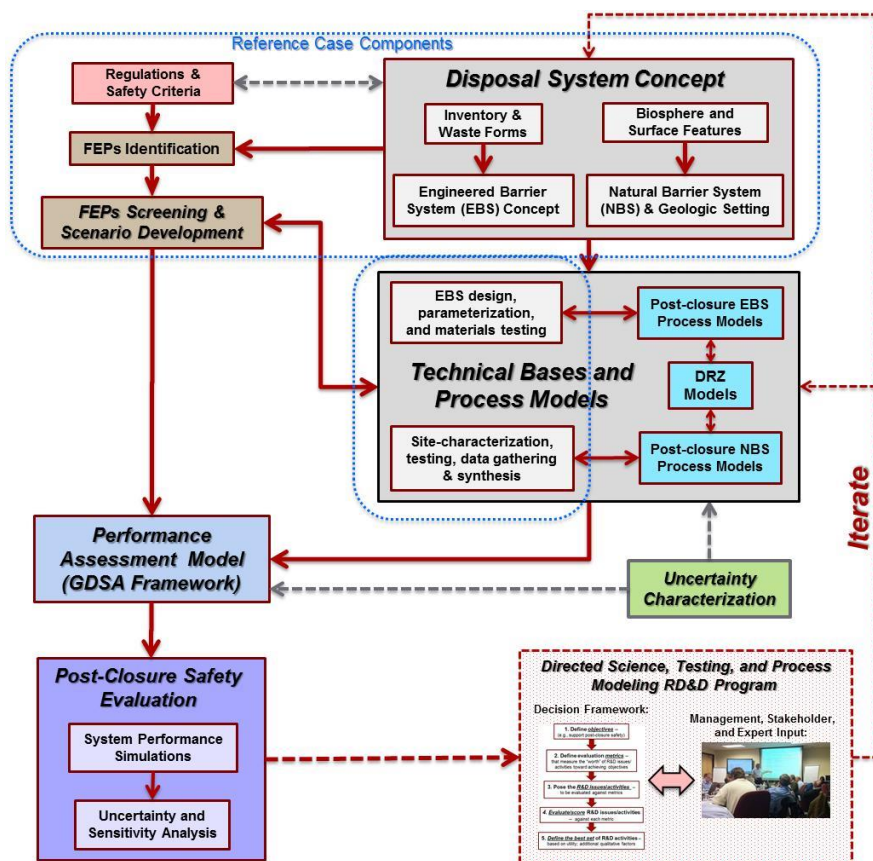


Fig. 3. Evolution and iteration of technical bases and performance assessment [8]. { Reference case components enclosed by blue dotted boxes. GDSA ≡ Geologic Disposal Safety Assessment. }

As noted by Vaughn et al. [9], the development of conceptual models for generic disposal systems has challenges: “Normally, a safety case and associated safety assessment address a specific site, a well-defined inventory, waste form, and waste package, a specific repository design, specific concept of operations, and an established regulatory environment. This level of specificity does not exist for a “generic” repository, so it is important to establish a reference case, to act as a surrogate for site/design specific information upon which a safety case can be developed. [A reference case provides] enough information to support the initial screening of FEPs [features, events, and processes] and the design of models for preliminary safety assessments...” The generic reference case for a DWR in crystalline (granitic) host rock is represented in Fig. 3 by the elements outlined with blue dotted lines. Characteristics and parameters associated with these reference-case components are discussed at length by Sevougian et al. [8], and summarized below. Additional detailed information about the reference case is provided by Sassani et al. [10] for inventory and waste characterization and by Matteo et al. [11] for engineered barrier system (EBS) design concepts.

Details of the “Performance Assessment Model (GDSA Framework)” box shown in Fig. 3 are discussed by Mariner et al. [12]. Development of an enhanced performance assessment (PA) capability for geologic disposal of SNF and HLW has been ongoing for several years in the U.S. repository program [13, 14], but has mainly been applied to evaluation of a repository for *commercial* SNF—a waste which generates significant decay heat that might strongly influence porewater movement and associated transport of released radionuclides. This enhanced PA capability, i.e., the *Geologic Disposal Safety Assessment (GDSA) Framework* (<https://pa.sandia.gov>) has now been applied to a much cooler defense waste

repository, as described herein. The *GDSA Framework* utilizes modern software and hardware capabilities and is based on open-source software architecture and configured to run in a massively parallel, high-performance computing (HPC) environment. It consists of two main components, the open-source Dakota uncertainty sampling and analysis software [15] and the PFLOTRAN multi-phase flow and reactive transport simulator [16, 17].

CRYSTALLINE HOST-ROCK REFERENCE CASE

All geologic media (e.g., crystalline, argillite, salt) are currently under consideration for a mined DWR [1, Sec. 3; 2, Sec. 3.1.2.2]. However, the reference case reported herein was developed concurrently with generic studies of a repository for commercial SNF in a mined crystalline concept [12]. Therefore, a crystalline concept was the first DWR reference case evaluated with *GDSA Framework*. A generic mined DWR in a bedded salt host rock was examined subsequently and has been reported in detail by Sevougian et al. [8], while a generic mined DWR in argillite is slated for future R&D. Generic repositories for *commercial* SNF in either bedded salt or argillite host rock have been investigated previously [13, 14]. The DWR crystalline host-rock reference case consists of a mined repository approximately half a kilometer below the surface in sparsely fractured crystalline host rock, such as granite or metagranite. Regionally, the topographic slope is less than 1 degree, and the water table is unconfined, a combination which would provide little driving force for deep fluid flow. The reference repository site has a stable cratonic terrain with low probabilities of seismicity, igneous activity, and human intrusion. The latter probability is reduced by avoiding regions with known geologic resources such as extensive fresh water aquifers, ore deposits, fossil fuels, or high geothermal heat flux (which offers the potential for geothermal development). This concept is consistent with international concepts of disposal in crystalline rock [18].

Characteristics of the crystalline host rock that contribute to or impact post-closure safety include [19, 20, 12]: (1) the high structural strength of the host rock, which stabilizes engineered barriers; (2) the depth of burial, which isolates the repository from surface processes (such as erosion and glaciation); (3) the low permeability of the host rock matrix, which isolates the repository from surface waters; (4) the reducing chemical environment, which lowers waste package corrosion rates (contributing to waste containment), limits radionuclide solubility, and enhances radionuclide sorption (limiting and delaying radionuclide transport); and (5) the potential presence of a fracture network that could create a hydraulic connection between the repository and the biosphere, which if present could adversely impact the isolation of the repository by enhancing the transport of released radionuclides. While the first and fifth characteristics are unique to crystalline rock, the second, third, and fourth characteristics generally apply to mined geologic repositories in any host rock (e.g., argillite and salt). But, it should also be noted that deep boreholes in crystalline rock are being considered for special types of defense waste [1].

The current crystalline reference case repository comprises a series of mined parallel disposal drifts (tunnels) connected by access halls. Repository access would be via vertical shafts and/or a ramp. Within the disposal drifts, multi-canister defense HLW (DHLW) waste packages^a are centered in a cylindrical buffer consisting of compacted bentonite pellets and/or bricks, as shown in Fig. 4. The bentonite buffer serves as an impermeable barrier to bulk movement of pore water, effectively isolating the waste container (and its radionuclide inventory) from connection with possible fractures in the host rock and the disturbed rock zone (DRZ) surrounding the drift excavation. If the buffer successfully fulfills its isolation safety function, the only mode of radionuclide transport from a breached waste package to the surrounding host rock is via the very slow process of molecular diffusion. This is the case for an undisturbed (nominal-evolution) scenario. For a disturbed scenario, such as human intrusion or glaciation, the potential effect of a disrupted buffer would be incorporated into the safety assessment.

^a The initial generic design envisions a corrosion-resistant waste-package overpack enclosing five stainless steel pour canisters containing borosilicate, vitrified HLW.

In order to explore another possible emplacement mode (besides multi-canister, horizontally emplaced DHLW waste packages), waste packages containing a single canister of thermally hotter defense SNF (DSNF) are emplaced in short vertical boreholes drilled beneath floors of DSNF disposal drifts, such as shown in Fig. 5. Each waste package sits on a plug of low permeability engineered material (assumed to be concrete) and is surrounded by low permeability engineered material (assumed to be compacted bentonite). DSNF drifts are also backfilled with low permeability engineered material, assumed to be compacted bentonite for the purposes of the post-closure PA reported herein. These two design concepts for vertical single-canister emplacement of hotter DSNF and horizontal in-drift multi-canister emplacement of cooler DHLW are similar to those recommended by Matteo et al. [11, Sec. 2.3]. The former design concept has many of the characteristics of the Swedish KBS-3V concept [21] and the latter has many of the characteristics of a Yucca Mountain co-disposal waste package [22].

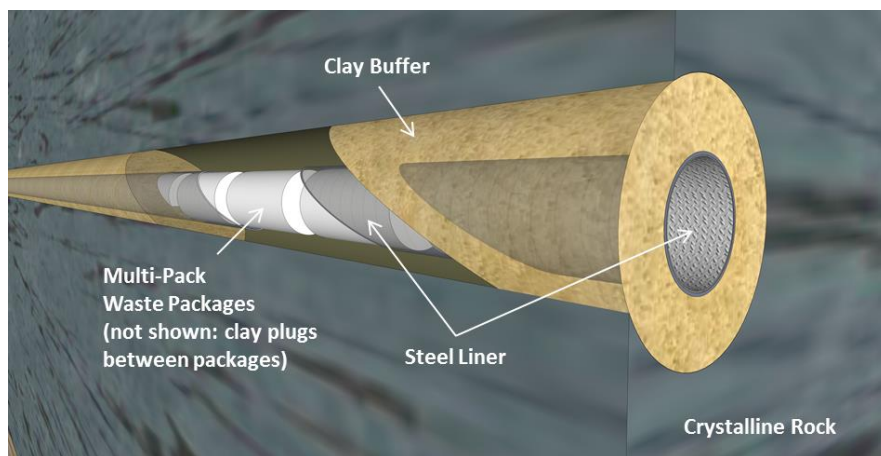


Fig. 4. Schematic of a disposal drift for a five-canister DHLW waste package in a generic crystalline host-rock repository [11].

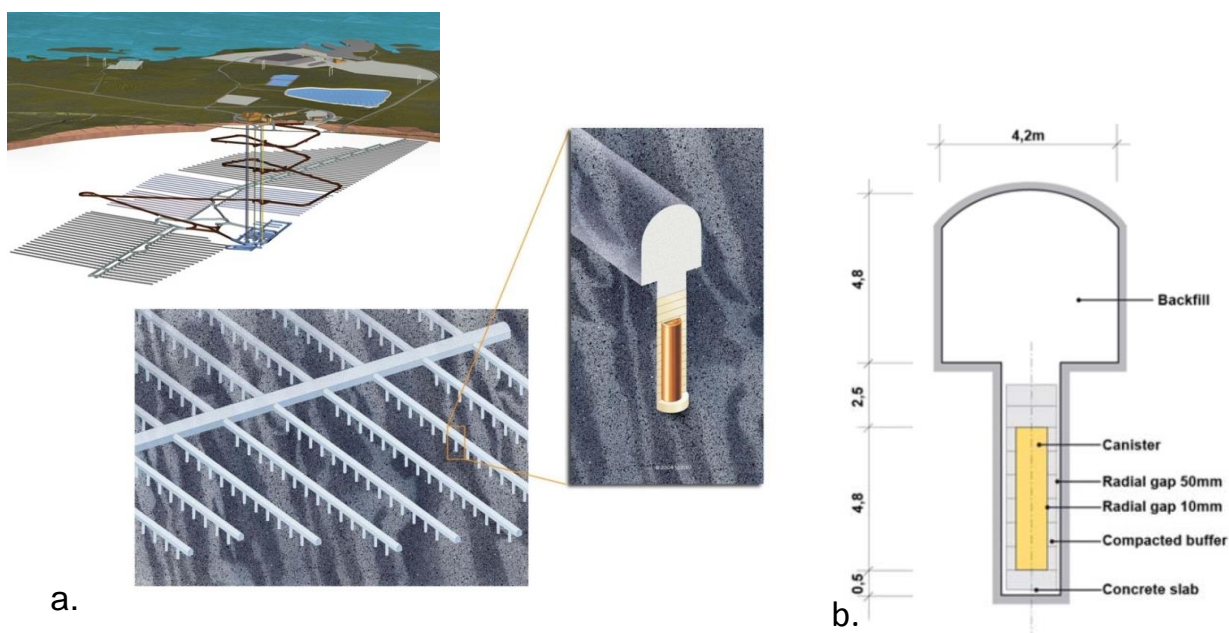


Fig. 5. Vertical emplacement concept similar to KBS-3V: (a) emplacement drifts and detail [23]; (b) placement of compacted bentonite buffer [24].

The reference-case radionuclide inventory is based on the glass DHLW inventories reported by Carter et al. [25] and DSNF inventories reported by Wilson [26]. It includes all projected DHLW glass at Hanford, all existing and projected DHLW glass at Savannah River, and all DSNF with a heat output of less than 1.5 kW/canister assuming 2010 wattages. At the time of disposal (assumed to be in 2038), heat output will be less than (or approximately equal to) 1 kW/canister for all types of waste. To calculate the radionuclide inventory per waste package for PA simulations, each bulk inventory was divided by the corresponding total number of canisters and multiplied by the number of canisters per waste package (e.g., five in the case of the DHLW generic disposal concept). Radionuclide inventories were then decayed as a function of time in order to calculate the heat of decay per waste package over time. Resulting curves are plotted in Fig. 5.

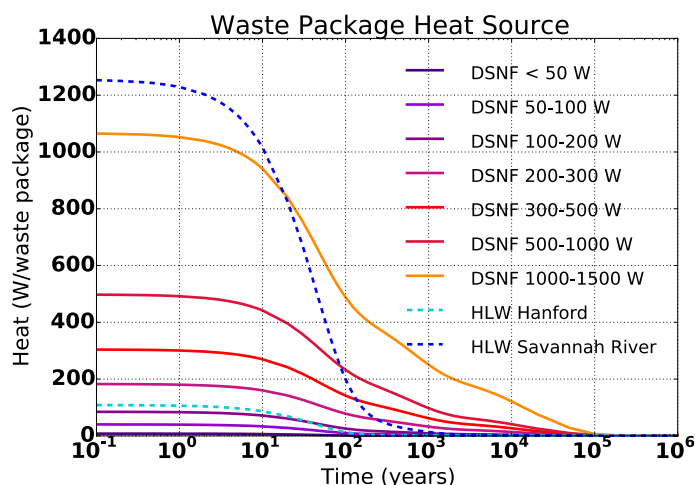


Fig. 5. Heat of decay versus time per waste package for the DSNF and glass DHLW included in the DWR PA simulations. [Time zero is the year 2038.]

Regarding the waste packages or disposal overpacks, the glass DHLW waste package is stainless steel and assumed to be similar in dimensions to the Yucca Mountain co-disposal package [22, Fig. 1.5.2-5], which is 2.1 m in diameter and either 3.7 m (short co-disposal package) or 5.3 m (long co-disposal package) in length. Each DHLW waste package contains five stainless steel pour canisters with vitrified borosilicate HLW in each canister. In the initial PA simulations, each waste package is a single region containing a radionuclide source term and a heat source term [8]. DSNF waste packages consist of corrosion-resistant overpacks with median lifetimes of about 45,000 years [8, Fig. 3-17], which each hold a single standardized DSNF canister [11, App. A]. Current PA simulations assume waste package dimensions identical to those of the large, long, standardized canister: 4.6 m in length and 0.61 m in diameter [22, Figure 1.5.1-9].

The representation of fractured crystalline rock in the generic reference case is based primarily on the well-characterized, sparsely fractured metagranite at Forsmark, Sweden [27, 28]. The Forsmark site is in the Fennoscandian Shield and consists of crystalline bedrock (primarily granite with lesser amounts of granodiorite, tonalite, and amphibolite) that formed between 1.89 and 1.85 Ga (1 Ga = 1 billion years), experienced ductile deformation and metamorphism, and cooled to the limit of brittle deformation between 1.8 and 1.7 Ga [29]. Crystalline basement with similar history exists within the United States [30]—see Fig. 6, and can be reasonably expected to have similar hydraulic properties. Conceptually, the crystalline host rock is comprised of two media: fractures and matrix. Numerically it is simulated in *GDSA Framework* with two types of grid cells: those containing a fracture or fractures and those without fractures (the matrix). Hydraulic parameters (permeability and porosity) describing fracture grid cells are

derived from fracture parameters developed for the Forsmark metagranite [27, 28, 31]. Hydraulic parameters describing matrix cells are derived from measurements made in tunnel walls of underground research laboratories (URLs) in crystalline rock at the Grimsel Test Site, Switzerland [32, 33], Lac du Bonnet batholith, Canada [34], and the Korean Underground Research Tunnel [35]. All other parameters are identical in fracture and matrix cells.

Host rock permeability due to fractures depends upon the distribution, orientation, and transmissivity of open, conductive fractures. Porosity due to fractures additionally depends on fracture aperture. Statistical descriptions of the foregoing fracture properties are used to generate multiple realizations of discrete fracture networks (DFNs), which are mapped to an equivalent continuous porous medium (ECPM) domain [12, Sec. 3.1.3.1], in which each grid cell intersected by a fracture or fractures is assigned a fracture-dependent anisotropic permeability and a fracture-dependent porosity [8, Sec. 3.2.2.1].

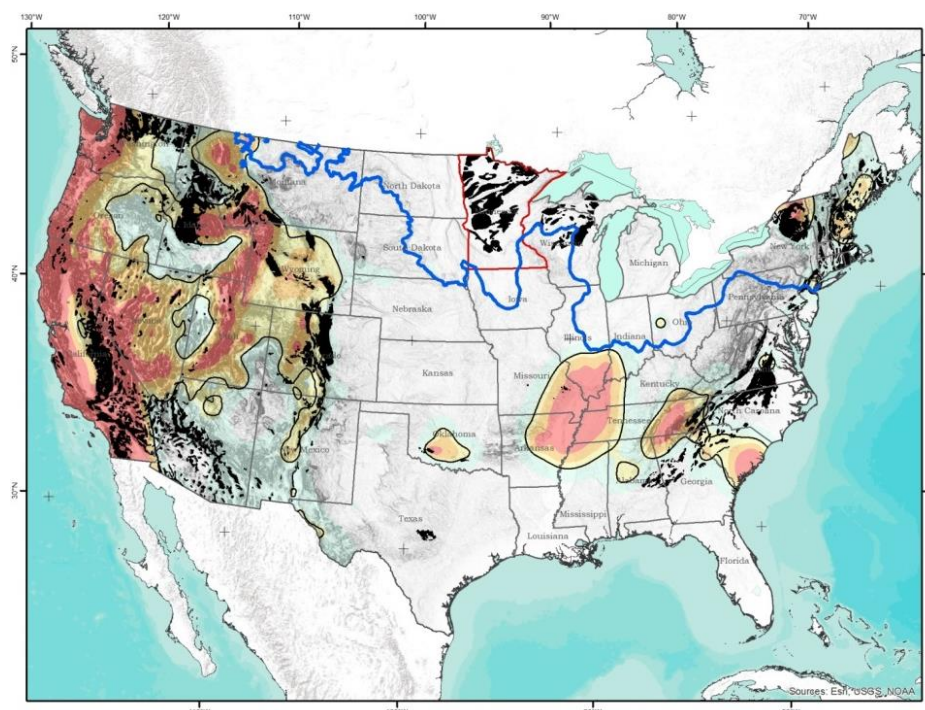


Fig. 6. Locations of crystalline rock outcrop and near-surface subcrop in the U.S. (black). Regions of high seismic hazard shown in warm color shading. Blue line is the maximum extent of the last glacial maximum [30, Fig. 2-2].

POST-CLOSURE PERFORMANCE ASSESSMENT SIMULATIONS

Conceptual and Numerical Model

The generic post-closure PA is currently focused on the undisturbed, nominal-evolution scenario (e.g., no human intrusion, seismicity, or glacial fluid influx), based on slow corrosion of the waste package and diffusive releases through the buffer. Because the generic PA does not presently consider the biosphere, the performance metric is maximum radionuclide concentration rather than dose. PA simulations, comprising 15 deterministic simulations (based on 15 different fracture maps), as well as a suite of 50 probabilistic simulations (based on a single fracture map) for uncertainty and sensitivity analyses, were implemented within the *Geologic Disposal Safety Assessment (GDSA) Framework* [36, 12]—<https://pa.sandia.gov>, which employs PFLOTRAN [16] for numerically solving the energy, flow, and transport equations and Dakota for probabilistic sampling and analysis [15]. Parallelization in PFLOTRAN is achieved through domain decomposition using the Portable Extensible Toolkit for

Scientific Computation (PETSc) [37]. PFLOTRAN is written in Fortran 2003/2008 and leverages state-of-the-art Fortran programming (i.e. Fortran classes, pointers to procedures, etc.) to support its object-oriented design. The Dakota toolkit is an analysis package for uncertainty quantification, sensitivity analysis, optimization, and calibration, for a parallel computing environment. The unstructured mesh was gridded with Cubit [38]. DFNs were generated with dfnWorks [39, 40] and mapped to an equivalent continuous porous medium with mapDFN.py [12].

The simulated repository domain is shown in Figs. 7 and 8. Fig. 7 is a transparent view colored by permeability. The three-dimensional structures inside the domain are the repository (colored gray rather than by permeability), the deterministic deformation zone (colored red due to its high permeability), and the largest fractures of a stochastically generated fracture network. Most of the domain is discretized into cells 15 m on a side, which makes a total of about 8.6 million cells—approximately 6.2 million of which are the smaller cells in and around the repository. Fig. 8 shows an x - z slice through the repository at the y -midpoint of the repository. The left half of the repository (21 drifts)—see Fig. 10—contains DSNF waste packages emplaced in 80 vertical boreholes per drift. The right half of the repository (21 drifts) contains DHLW glass emplaced in 119 waste packages per drift. These DHLW drifts are filled first with Hanford-glass waste packages, followed by Savannah-River-glass waste packages. Details on initial and boundary conditions are described by Sevougian et al. [8], including the head gradient of -0.0013 m/m from west to east (left to right) across the domain.

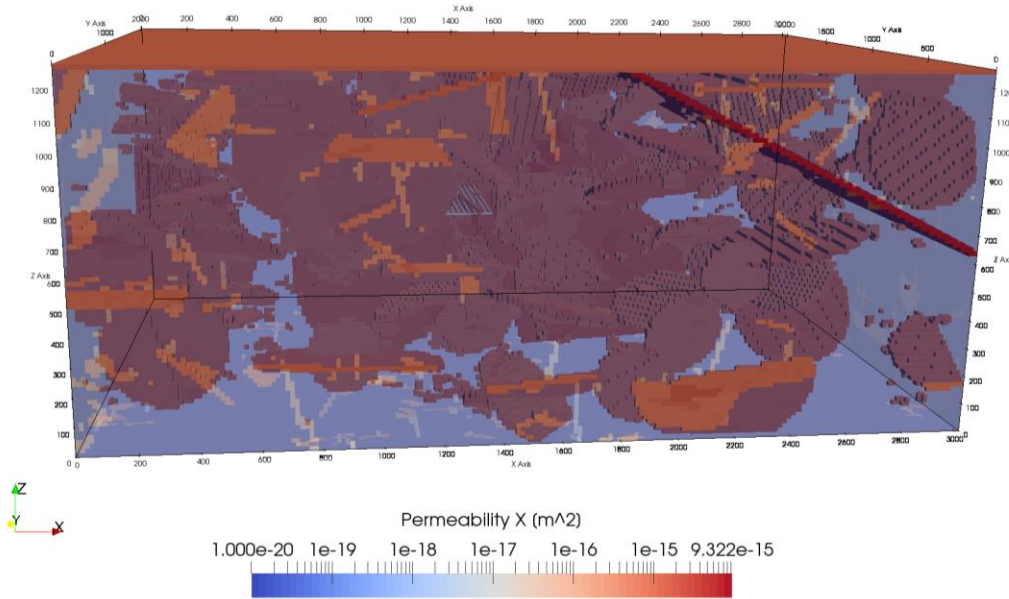


Fig. 7. Transparent view of the model domain colored by permeability. [Several repository drifts (colored gray) can be seen in the center of the figure.]

Fifteen fracture maps were generated for examining the effects of spatial variability (stochastic uncertainty) in the crystalline reference case. Each fracture-map realization also contains a single deterministic deformation zone striking north-south with a dip of 30° and a transmissivity of 1.5×10^{-6} m²/s. The current PA simulations are biased toward greater fracture connectivity than is observed at Forsmark [12, 27], in order to test some of the mapping features of the ECPM representation, and are therefore a conservative representation of repository performance in fractured crystalline host rock.

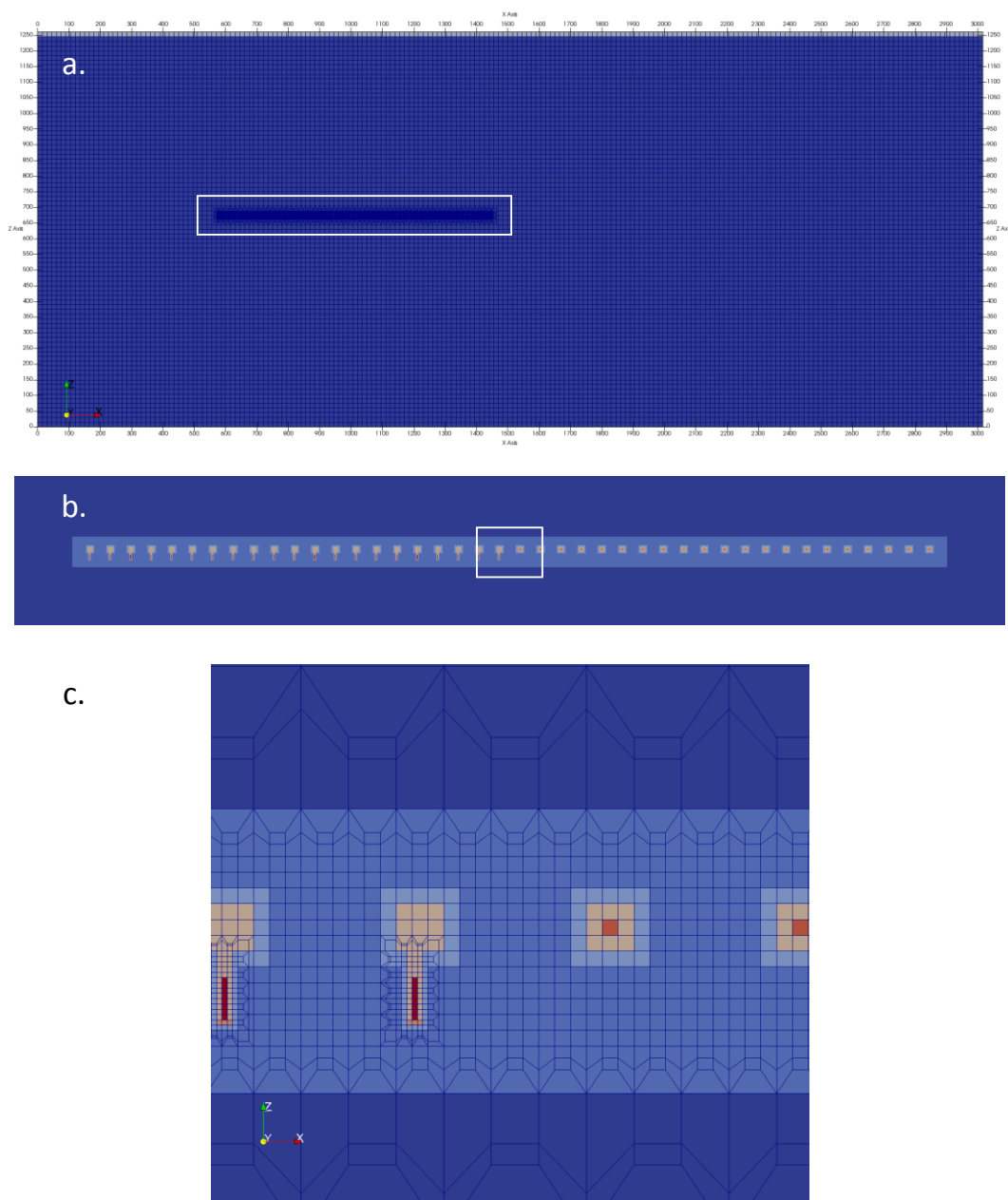


Fig. 8. X-Z slice of model domain. (a) Most of the domain is discretized with cells 15-m on a side. White box in (a) shows area of (b), in which DSNF drifts (left) and DHLW drifts (right) can be seen. White box in (b) shows area of (c), in which discretization of the repository (to 5/3 m (DHLW) and 5/9 m (DSNF)) can be seen. Colors represent materials: dark blue and medium blue, undisturbed host rock; light blue, DRZ; tan, buffer; light orange, cement; dark orange, DHLW; red, DSNF; grey, sediment [top of (a)].

Deterministic Simulation Results

Both deterministic and probabilistic results are discussed in terms of concentrations of the long-lived radionuclide I-129 ($t_{1/2} = 1.57 \times 10^7$ yr).^b I-129 is assumed to have unlimited solubility and to be non-sorbing; it thus behaves conservatively. Material properties used in the PA simulations are

^b Transport of the long-lived, moderately sorbing, and less soluble Np-237 is also depicted by Sevougian et al. [8].

summarized in TABLE 1 (deterministic parameter values) and TABLE 2 (sampled parameter ranges). Temperature fields and fluid flux vectors for a single deterministic simulation are also presented below.

For the deterministic simulation (based on a single fracture map, “Domain6”), Fig. 9 shows resulting waste package temperature histories for each of the two primary EBS design concepts under consideration here: vertical borehole emplacement of a waste package with a single canister of DSNF and horizontal emplacement of a much larger waste package containing five canisters of DHLW. For each of the two designs, Fig. 9 shows two temperature extremes for each type of waste package: (a) a relatively cool DSNF bin (100-200W single canisters) and the hottest DSNF bin (1000-1500W single canisters); and (b) the coolest DHLW (Hanford glass) and hottest DHLW (Savannah River glass), both emplaced as five canisters per waste package.

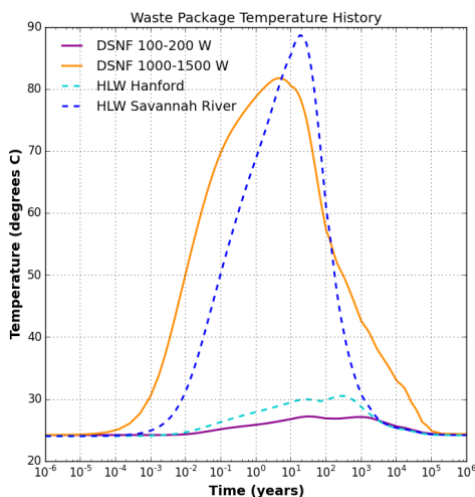


Fig. 9. Waste package temperature histories for two DSNF thermal bins (a cooler bin and the hottest bin), and the hottest and coolest DHLW for the generic DWR in crystalline host rock.

TABLE 1. Parameter values used in deterministic simulations.

Model Region	Permeability (m ²)	Porosity, ϕ	Tortuosity ^a , τ	Effective Diffusion Coefficient ^b , D_e (m ² /s)	Saturated Thermal Conductivity (W/m/K)	Heat Capacity (J/kg/K)
Waste Package	1×10^{-16}	0.50	1	5×10^{-10}	16.7	466
Bentonite Buffer	1×10^{-20}	0.35	0.35	1.225×10^{-10}	1.5	830
Crystalline Matrix	1×10^{-20}	0.005	0.2	1×10^{-12}	2.5	830
Fractures	Calc'd ^c	Calc'd ^c	Calc'd ^c	1×10^{-12}	2.5	830
DRZ	1×10^{-16}	0.01	1	1×10^{-11}	2.5	830
Sediments	1×10^{-15}	0.20	0.20	4×10^{-11}	1.7	830

^a Tortuosity as used in PFLOTRAN is defined by Sevougian et al. [8, App. B.]

^b $D_e = D_w \phi \tau s$, where s is the liquid saturation, assumed here to be = 1, and D_w is the free water diffusion coefficient = 1×10^{-9} m²/s [41].

^c Calculated on a cell by cell basis for each fracture realization—see [8, Table 3-10].

At one year after closure (or post-waste-emplacement—all waste is assumed to be emplaced simultaneously at time 0), increases in temperature associated with the Savannah River HLW and the warmer DSNF bins are apparent, and fluid fluxes associated with rising temperatures are established

[8, Fig. 3-10]. Peak repository temperatures occur at approximately 20 years (Fig. 10), with temperatures in the Savannah River HLW drifts being slightly less than 90°C (see also Fig. 9). Darcy flux vectors (in the ECPM domain) at 20 years are shown in Fig. 11, indicating a buoyant outflow of heated pore fluid from the warming repository. By 1,000 years repository temperatures have returned to near background, and the thermal influence on the flow field is diminished [8, Fig. 3-13].

TABLE 2. Sampled parameters and their distributions.

Parameter	Range	Units	Distribution
Glass exposure factor (f_e)	4 – 17 (mode = 4)		triangular
Mean Waste Package Degradation Rate	$10^{-5.5} - 10^{-4.5}$	yr ⁻¹	log uniform
Waste Package τ	0.01 – 1.0		log uniform
Bentonite ϕ	0.3 – 0.5		uniform
DRZ ϕ	0.005 – 0.05		uniform
Np K_d bentonite	0.1 – 702	m ³ kg ⁻¹	log uniform
Np K_d natural barrier	0.047 – 20	m ³ kg ⁻¹	log uniform

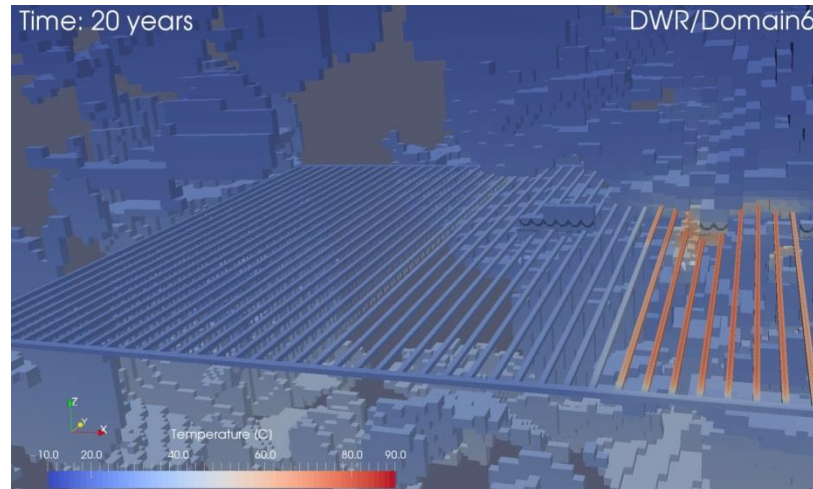


Fig. 10. Repository temperature field at 20 years in the deterministic simulation of fracture Domain6.

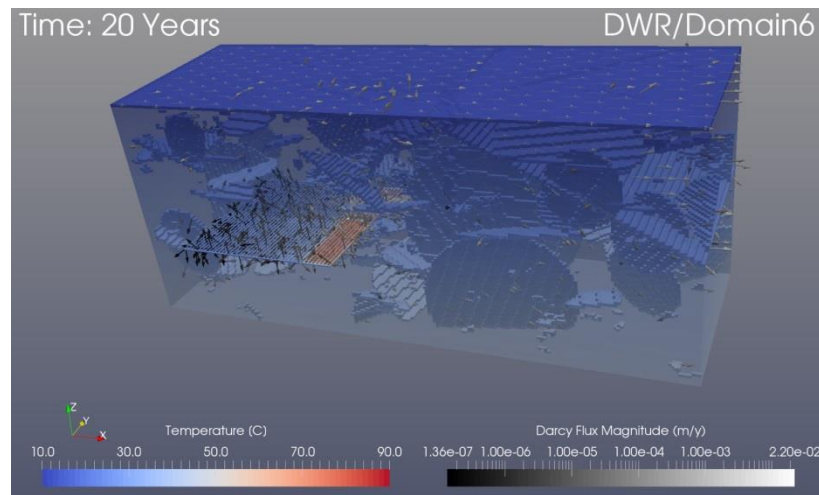


Fig. 11. Darcy fluid flux vectors at 20 years in the deterministic simulation of fracture Domain6.

Potential radionuclide releases from the repository depend not only on fluid fluxes, but on the timing of waste package breach and the resultant waste form degradation. The DSNF waste form is assumed to degrade instantaneously upon breach of the waste package [8, Sec. 3.1.3.2]. The DHLW waste form degrades exponentially [8, Sec. 3.1.3.1] after breach of the waste package. The spatial distribution of I-129 mobilized from the waste forms is shown in Figs. 12 and 13, at the post-closure times of 2,000 and 100,000 years, respectively. Between 1000 and 2000 years, some waste packages have failed (~10%) [8, Fig. 3-17], and by 2000 years radionuclide transport in fractures carries I-129 at dilute (10^{-12} mol/L) concentrations to the east (right) face of the model domain over 1.5 km from the repository (Fig. 12). With time, I-129 diffuses from the repository and from fractures into the crystalline rock matrix (Fig. 13).

Breakthrough curves for I-129 at three observation points in the surficial sediment (“glacial1”, “glacial2”, and “glacial3”) and three observation points in the deformation zone (“dz1”, “dz2”, and “dz3”) (see Fig. 14) have been compared [8] for the 15 deterministic simulations represented by the 15 fracture-map realizations. Among the various fracture-map realizations, the spread in time of earliest arrival (taken to be the time at which a concentration of 10^{-19} mol/L is reached) is approximately two orders of magnitude—between thousands and hundreds-of-thousands of years at each sediment observation point (Fig. 15). At which of the three observation points I-129 first arrives for any given fracture map depends on the randomly generated fracture connectivity for that given map. This is demonstrated in Fig. 15 by the dashed line, which indicates a deterministic simulation where I-129 arrived at the two furthest points from the repository first (approximately 20,000 years into the simulation) and at the closest observation point over 100,000 years later. At all observation points, the spread in maximum concentration of I-129, C_{I-129}^{max} , is approximately four orders of magnitude. The time of earliest arrival at any given point in the domain depends heavily on the connectivity (or lack thereof) between that point and the repository.

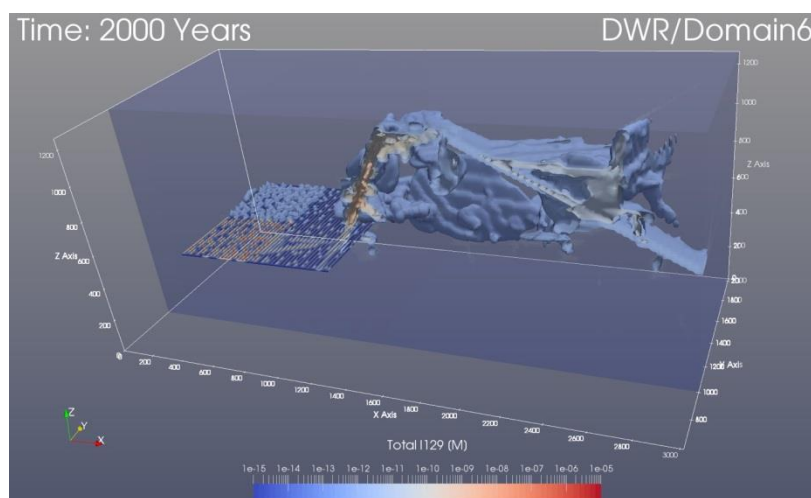


Fig. 12. I-129 concentration at 2000 years in the deterministic simulation of fracture Domain6.

Probabilistic Simulation Results

A suite of 50 simulations, based on 50 random samples (Latin hypercube sampling) of the parameter distributions listed in TABLE 2, was run to 1,000,000 years post-closure, but using the same fracture realization (Domain6) for each simulation. Concentrations were observed at the same observation points used to compare fracture realizations (Fig. 14). Mean breakthrough curves for all simulated radionuclides are plotted in Fig. 16 for the sediment (glacial till) observation points—each point on a mean breakthrough curve is an average at that time of the 50 concentration values for the given radionuclide. “Horsetail” plots of the 50 breakthrough curves for I-129 are plotted in Fig. 17. Predicted concentrations

of I-129 vary less due to the sampled parameters in TABLE 2 than due to variations in flow paths among fracture realizations (cf. Fig. 15 to Fig. 17). Similarly, the variation in maximum concentration of I-129 is much less over these probabilistic simulations for Domain6 than the variation across fracture realizations discussed in the previous section.

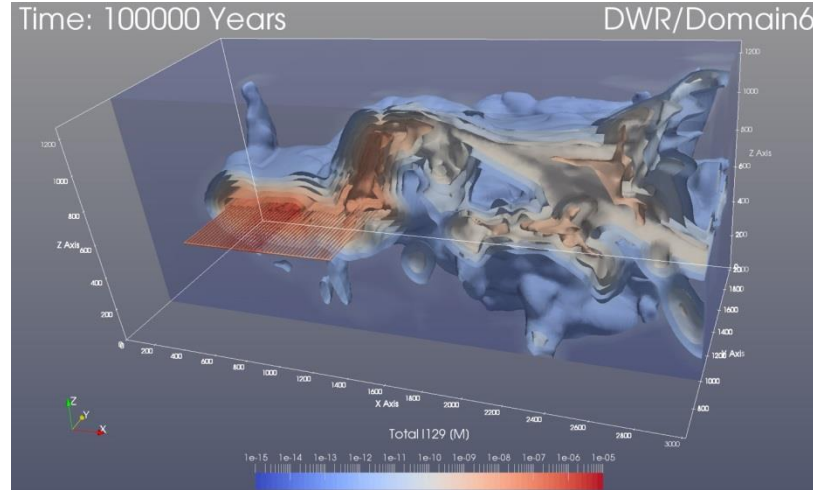


Fig. 13. I-129 concentration at 100,000 years in the deterministic simulation of fracture Domain6.

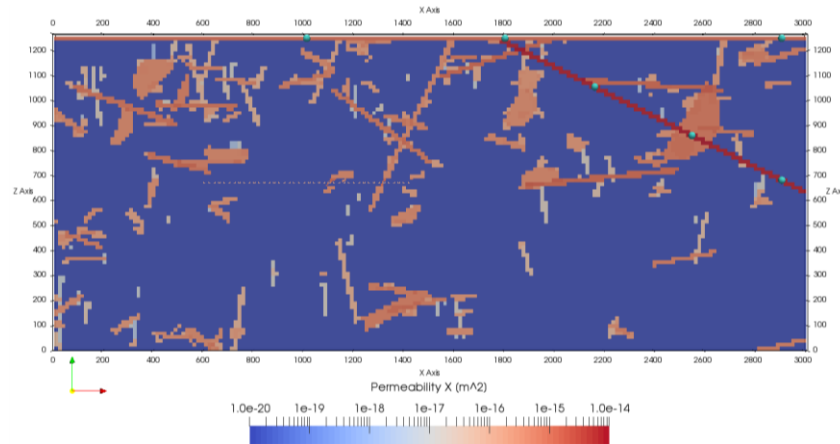


Fig. 14. X-Z cross section at the Y midpoint of the domain showing the locations of observation points (teal spheres) used in comparison of fracture maps and in sensitivity analysis. From left to right in uppermost layer (sediments): “glacial1,” “glacial2,” and “glacial3.” From top to bottom in deformation zone: “dz1,” “dz2,” “dz3.”

Scatter plots and Spearman’s rank correlation coefficients (SRCCs) [8, 42] were calculated in order to assess the sensitivity of C_{I-129}^{max} to sampled input parameters. As might be expected from the narrow spread of the individual breakthrough curves in Fig. 17, these sensitivity analysis techniques showed few significant correlations. This can be attributed primarily to the very fast transport through fractured rock. The only uncertain parameter that showed significant correlation was “Glacial seds k ” (or permeability in the glacial-till sediment at the top of the domain). This is indicated in Fig. 18, which shows both the scatter plot for C_{I-129}^{max} versus “Glacial seds k ” and the SRCC plot for all the uncertain parameters in TABLE 2. The SRCC shows a positive correlation, which is misleading because the scatter plot indicates that the SRCC should be positive over the lower end of the permeability range, but negative over the upper end. The positive correlation at the low end is simply because C_{I-129}^{max} over 1,000,000 years is the I-129 value exactly at 1,000,000 years, when the curve still has not reached its peak (i.e., only the leading edge of the plume has broken through). The negative correlation at the higher end of the permeability

range is because the higher the permeability, the higher the fluid flow rate; and, thus, the more the I-129 plume is diluted when it transfers from the granite fracture domain to the upper glacial sediment domain. This is a good demonstration of why more than one sensitivity analysis technique is generally necessary to understand a model representing multiple processes.

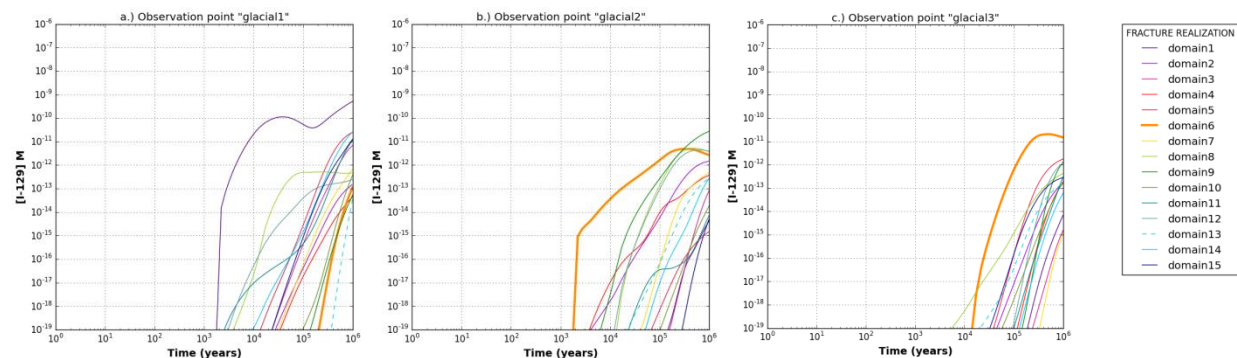


Fig. 15. Predicted concentration of I-129 versus time for 15 fracture-map realizations at various observation points in the surficial sediments (glacial till).

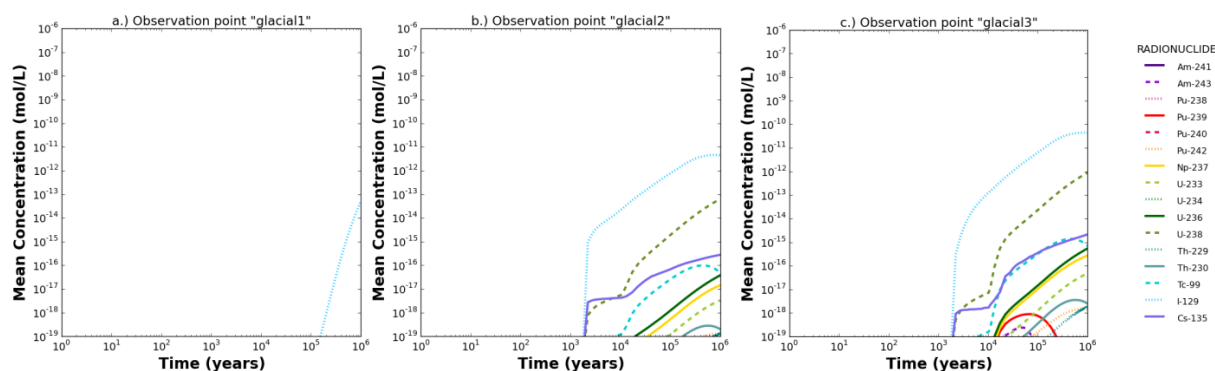


Fig. 16. Mean concentrations of all simulated radionuclides, predicted on the basis of 50 realizations.

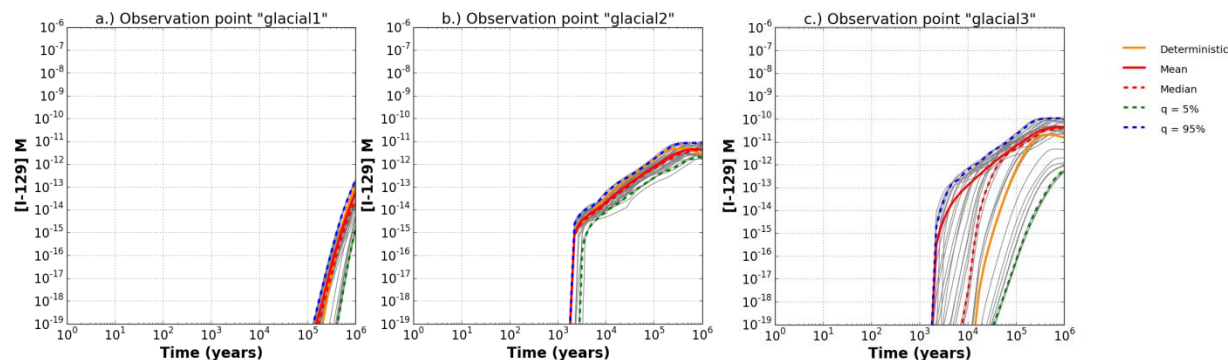


Fig. 17. Predicted concentration of I-129 versus time at three sediments observation points, for 50 realizations of the uncertain parameters. [The heavy orange line is the deterministic simulation of fracture Domain6.]

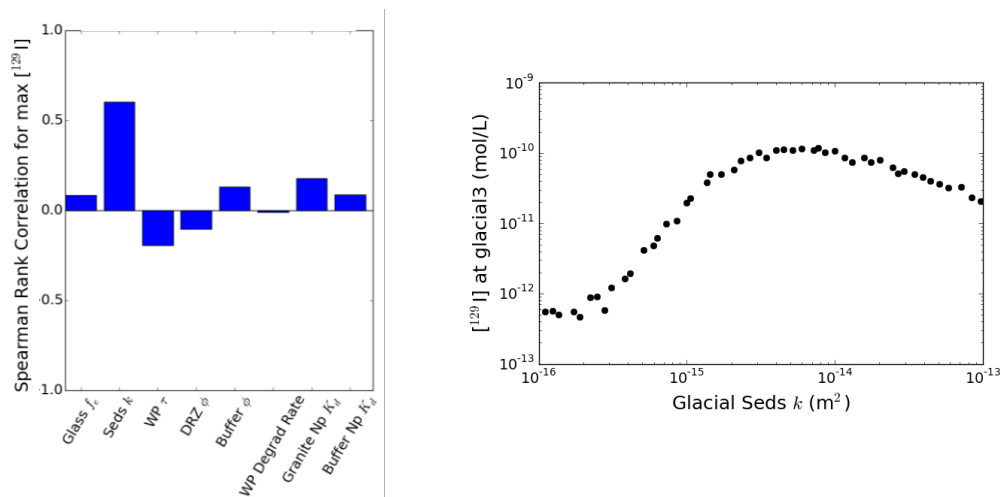


Fig. 18. Spearman's rank correlation coefficients for maximum I-129 concentration versus sampled input parameters (left); and scatter plot of maximum I-129 concentration versus permeability in glacial sediments (right). Plotted at the "glacial3" observation point.

SUMMARY AND CONCLUSIONS

Recently the U.S. made a policy decision to begin R&D for geologic disposal of defense-related HLW/SNF in a facility separate from commercially generated waste. A deep geologic repository for the disposal of DOE-managed HLW, and some thermally cooler DOE-managed SNF, arising from defense and DOE R&D activities, is part of a stepwise, phased approach for disposal of the Nation's nuclear waste, as recommended by the Blue Ribbon Commission on America's Nuclear Future. The work discussed here is the beginning of an R&D effort that focuses on post-closure safety (or performance) assessment for such a Defense Waste Repository (DWR). The major components of the safety assessment are: (1) development of generic reference cases (i.e., knowledge or technical bases for "generic" or "non-site-specific" deep geologic repositories); (2) features, events, and processes (FEPs) analyses and screening to support the technical bases and performance assessment (PA) model; (3) performance evaluation of alternative EBS design concepts; and (4) post-closure safety analysis of the repository system under consideration.

Using the known inventory of defense-related SNF, as well as defense-related HLW stored at the Savannah River and Hanford sites, the *Geologic Disposal Safety Assessment (GDSA) Framework* modeling and software system has been applied to simulate the potential performance of a DWR in a fractured crystalline host rock, resulting in a suite of single-realization (i.e., deterministic) and multi-realization (i.e., probabilistic) 3-D post-closure system analyses, over a performance period of one million years. Two types of emplacement concepts are examined, including single-canister vertical-borehole emplacement for the hotter defense SNF waste (KBS-3V concept) and multi-canister horizontal emplacement for defense HLW (similar to Yucca Mountain co-disposal waste packages). Sensitivity analyses examine the effect of key uncertain parameters on repository performance, including the effects of fracture distribution, waste package degradation rate, buffer and disturbed rock zone (DRZ) properties, and sorption parameters. Such analyses are part of an iterative decision-making process that determines the current technical maturity of key system elements and then focuses future R&D on parameters and processes with the highest uncertainty. They also help during the repository siting process by providing a method to assess the relative maturity and potential performance of candidate sites.

The current crystalline-rock PA simulations are biased toward greater fracture connectivity, in order to test some of the mapping features of the equivalent continuous porous medium (ECPM) representation,

and are therefore a conservative representation of repository performance in fractured crystalline host rock. Also, fractured media present new challenges in uncertainty and sensitivity analysis, which might be addressed through introduction of a performance metric other than concentration (or dose) at a specific point location—for example, a metric that averages concentrations over a set of withdrawal wells. Initial results indicate that a crystalline host rock with a connected fracture system may require additional safety features to ensure robustness of the isolation safety function, such as a deep unsaturated zone, a sufficiently thick sedimentary overburden, and/or a disposal overpack with a very slow corrosion rate. None of these should pose an undue obstacle for successful disposal.

REFERENCES

1. DOE (U.S. Department of Energy) 2014. *Assessment of Disposal Options for DOE-Managed High-Level Radioactive Waste and Spent Nuclear Fuel*, October 2014.
2. DOE (U.S. Department of Energy) 2015. *Report on Separate Disposal of Defense High-Level Radioactive Waste*, March 2015.
3. GAO (U.S. Government Accountability Office) 2017. *Benefits and Costs Should Be Better Understood Before DOE Commits to a Separate Repository for Defense Waste*, GAO-17-174, Jan. 2017.
4. DOE (U.S. Department of Energy) 2010. *Program and Project Management for the Acquisition of Capital Assets*, DOE O 413.3B, 11-29-2010, U.S. Department of Energy, Washington, D.C. 20585, available at <https://www.directives.doe.gov/directives-documents/400-series/0413.3-BOrder-b>
5. DOE (U.S. Department of Energy) 2011. *Technology Readiness Assessment Guide*, DOE G 413.3-4A, 9-15-2011, U.S. Department of Energy, Washington, D.C. 20585, www.directives.doe.gov
6. Sevougian, S. D., G. Freeze, M. Gross, K. Kuhlman, C. Leigh, J. Wolf, D. Buhmann, and J. Mönig 2016. “Joint US-German FEPs Catalog,” presented at the 7th US/German Workshop on Salt Repository Research, Design, and Operation, Washington, DC, September 7-9, 2016, SAND2016-8441C, Sandia National Laboratories, Albuquerque, NM.
7. Sevougian, S. D. 2016. “Application of the Technology Readiness Assessment (TRA) Process to Deep Geologic Repository Systems,” presented at the 2nd DAEF Conference on Key Topics in Deep Geological Disposal, Cologne, Germany, September 27-28, 2016, SAND2016-9353C, Sandia National Laboratories, Albuquerque, NM.
8. Sevougian, S. D., E. R. Stein, M. B. Gross, G. E. Hammond, J. M. Frederick, and P. E. Mariner 2016. *Status of Progress Made Toward Safety Analysis and Technical Site Evaluations for DOE Managed HLW and SNF*. SAND2016-11232R; FCRD-UFD-2016-000082, Rev. 1. Sandia National Laboratories, Albuquerque, NM.
9. Vaughn, P., S. D. Sevougian, E. L. Hardin, P. Mariner, and M. B. Gross 2013. “Reference Case For Generic Disposal of HLW and SNF in Salt,” in *Proceedings of the 2013 International High-Level Radioactive Waste Management Conference*, Albuquerque, NM, April 28 – May 2, 2013, American Nuclear Society, La Grange Park, IL. (www.ans.org)
10. Sassani, D. C., J.-H. Jang, P. Mariner, L. Price, R. P. Rechard, M. Rigali, R. Rogers, E. R. Stein, W. Walkow, and P. F. Weck 2016. *The On-line Waste Library (OWL): Usage and Inventory Status Report*. SAND2016-9485 R; FCRD-UFD-2016-000080. Sandia National Laboratories, Albuquerque, NM.
11. Matteo, E., E. Hardin, T. Hadgu, H. Park, M. Rigali, and C. F. Jove-Colon 2016. *Status of Progress Made Toward Preliminary Design Concepts for the Inventory in Select Media for DOE-Managed HLW/SNF*. SAND2016-9823 R; FCRD-UFD-2016-000081. Sandia National Laboratories, Albuquerque, NM.
12. Mariner, P. E., E. R. Stein, J. M. Frederick, S. D. Sevougian, G. E. Hammond, and D. G. Fascitelli 2016. *Advances in Geologic Disposal System Modeling and Application to Crystalline Rock*, FCRD-UFD-2016-000440, SAND2016-96107R. Sandia National Laboratories, Albuquerque, NM, September 22, 2016.
13. Sevougian, S. D., G. A. Freeze, W. P. Gardner, G. E. Hammond, P. Mariner, and R. J. MacKinnon. 2015. “Performance Assessment Modeling of a Generic SNF/HLW Repository in Salt with Coupled Thermal-Hydrologic Effects – 15423,” in *Proceedings of the WM2015 Conference*, March 15 – 19, 2015, Phoenix, Arizona USA.
14. Sevougian, S. D., E. R. Stein, G. E. Hammond, P. E. Mariner, and W. P. Gardner 2016. “Enhanced Performance Assessment Models for Generic Deep Geologic Repositories for High-Level Waste and Spent Nuclear Fuel – 16223,” in *Proceedings of the WM2016 Conference*, March 6 – 10, 2016, Phoenix, Arizona USA.

15. Adams, B.M., M.S. Ebeida, M.S. Eldred, J.D. Jakeman, K.A. Maupin, J.A. Monschke, L.P. Swiler, J.A. Stephens, D.M. Vigil, T.M. Wildey, W.J. Bohnhoff, K.R. Dalbey, J.P. Eddy, R.W. Hooper, K.T. Hu, P.D. Hough, E.M. Ridgway, A. Rushdi 2016. *Dakota, a Multilevel Parallel Object-Oriented Framework for Design Optimization, Parameter Estimation, Uncertainty Quantification, and Sensitivity Analysis: Version 6.4 User's Manual*. SAND2014-4633, July 2014, Updated May 9, 2016. Sandia National Laboratories, Albuquerque, NM. (<http://dakota.sandia.gov/>)
16. Hammond, G.E., P.C. Lichtner and R.T. Mills 2014. "Evaluating the Performance of Parallel Subsurface Simulators: An Illustrative Example with PFLOTTRAN", *Water Resources Research*, 50, doi:10.1002/2012WR013483.
17. Lichtner, P. C., G. E. Hammond, C. Lu, S. Karra, G. Bisht, B. Andre, R. Mills, and J. Kumar 2015. *PFLOTTRAN User Manual: A Massively Parallel Reactive Flow and Transport Model for Describing Surface and Subsurface Processes*, http://www.pfлотran.org/docs/user_manual.pdf, January 20, 2015
18. SKB (Svensk Kärnbränslehantering AB) 2007. *Geology Forsmark*. R-07-45 Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.
19. Mariner, P., J. H. Lee, E. Hardin, F. D. Hansen, G. Freeze, A. S. Lord, B. Goldstein, and R. H. Price 2011. *Granite Disposal of U.S. High-Level Radioactive Waste*. SAND2011-6203. Sandia National Laboratories, Albuquerque, NM.
20. Freeze, G., M. Voegelé, P. Vaughn, J. Prouty, W.M. Nutt, E. Hardin, and S.D. Sevougian 2013. *Generic Deep Geologic Disposal Safety Case*. FCRD-UFD-2012-000146 Rev. 1, SAND2013-0974P, August 2013, Sandia National Laboratories, Albuquerque, NM.
21. SKB (Svensk Kärnbränslehantering AB) 2011. *Long-term safety for the final repository for spent nuclear fuel at Forsmark: Main report of the SR-Site project* (3 volumes). TR-11-01. Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden. (www.skb.se/publications)
22. DOE (U.S. Department of Energy) 2008. *Yucca Mountain Repository License Application Safety Analysis Report*. DOE/RW-0573, Revision 1. U.S. Department of Energy, Washington, DC. (<http://www.nrc.gov/waste/hlw-disposal/yucca-lic-app/yucca-lic-app-safety-report.html#1>)
23. Kempainen K. 2014. "Case Study: ONKALO Underground Rock Characterization Facility," in *Proceedings of the IAEA Workshop on Need for and Use of Generic and Site-Specific Underground Research Laboratories to Support Siting, Design and Safety Assessment Developments*, Oct. 7-9, 2014, Albuquerque, NM, http://connect.iaea.org/sites/connect-members/URF/2014-URF-Use_SandiaVenue/default.aspx
24. Pettersson, S. and B. Lönnerberg. (2008). *Final Repository for Spent Nuclear Fuel in Granite - The KBS-3V Concept in Sweden and Finland*. Paper presented at the International Conference Underground Disposal Unit Design & Emplacement Processes for a Deep Geologic Repository, Prague.
25. Carter, J. T., A. J. Luptak, J. Gastelum, C. Stockman, and A. Miller 2013. *Fuel Cycle Potential Waste Inventory for Disposition*. FCRD-USED-2010-000031 Rev 6. Savannah River National Laboratory, Aiken, SC.
26. Wilson, J. 2016. *Decay Heat of Selected DOE Defense Waste Materials*, FCRD-UFD-2016-000636, SRNL-RP-2016-00249, Savannah River National Laboratory, Aiken, SC.
27. Follin, S., L. Hartley, I. Rhen, P. Jackson, S. Joyce, D. Roberts, and B. Swift 2014. "A methodology to constrain the parameters of a hydrogeological discrete fracture network model for sparsely fractured crystalline rock, exemplified by data from the proposed high-level nuclear waste repository site at Forsmark, Sweden," *Hydrogeology Journal*, 22(2), 313-331. doi: 10.1007/s10040-013-1080-2
28. Joyce, S., L. Hartley, D. Applegate, J. Hoek, and P. Jackson 2014. "Multi-scale groundwater flow modeling during temperate climate conditions for the safety assessment of the proposed high-level nuclear waste repository site at Forsmark, Sweden". *Hydrogeology Journal*, 22(6), 1233-1249.
29. SKB (Svensk Kärnbränslehantering AB) 2007. *Geology Forsmark*. R-07-45 Swedish Nuclear Fuel and Waste Management Co., Stockholm, Sweden.
30. Perry, F. V., R. E. Kelley, and D. M. Milazzo 2016. *Regional Geologic Evaluations for Disposal of HLW and SNF: Archean Crystalline Rocks of the North-Central United States*. FCRD-UFD-2016-000634; LA-UR-16-27845. Los Alamos National Laboratory, Los Alamos, NM.
31. Wang, Y., et al. 2014. *Used Fuel Disposal in Crystalline Rocks: Status and FY14 Progress*, FCRD-UFD-2014-000060, SAND2014-17992R, Sandia National Laboratories, Albuquerque, New Mexico, September 2014.
32. Schild, M., S. Siegesmund, A. Vollbrecht, and M. Mazurek 2001. "Characterization of granite matrix porosity and pore-space geometry by in situ and laboratory methods". *Geophysical Journal International*, 146(1), 111-125. doi: 10.1046/j.0956-540x.2001.01427.x
33. Soler, J. M., J. Landa, V. Havlova, Y. Tachi, T. Ebina, P. Sardini, M. Siitari-Kauppi, J. Eikenberg, and A. J. Martin 2015. "Comparative modeling of an in situ diffusion experiment in granite at the Grimsel Test Site".

- Journal of Contaminant Hydrology*, 179, 89-101. doi: 10.1016/j.jconhyd.2015.06.002
34. Martino, J. B. and N. A. Chandler 2004. "Excavation-induced damage studies at the Underground Research Laboratory". *International Journal of Rock Mechanics and Mining Sciences*, 41(8), 1413-1426.
 35. Cho, W.-J., J.-S. Kim, C. Lee, and H.-J. Choi 2013. "Gas permeability in the excavation damaged zone at KURT". *Engineering Geology*, 164, 222-229. doi: 10.1016/j.enggeo.2013.07.010
 36. Mariner, P. E., W. P. Gardner, G. E. Hammond, S. D. Sevougian, and E. R. Stein 2015. *Application of Generic Disposal System Models*. SAND2015-10037 R; FCRD-UFD-2015-000126. Sandia National Laboratories, Albuquerque, NM.
 37. Balay S., J. Brown, K. Buschelman, V. Eijkhout, W.D. Gropp, D. Kaushik, M.G. Knepley, L. Curfman McInnes, B.F. Smith and H. Zhang 2013. *PETSc Users Manual*, ANL-95/11 – Revision 3.4, Argonne National Laboratory, Argonne IL.
 38. Blacker, T., S. J. Owen, M. L. Staten, R. W. Quador, B. Hanks, B. Clark, R. J. Meyers, C. Ernst, K. Merkley, R. Morris, C. McBride, C. Stimpson, M. Plooster, and S. Showman 2016. *CUBIT Geometry and Mesh Generation Toolkit 15.2 User Documentation*. Sandia National Laboratories, Albuquerque, NM.
 39. Hyman, J. D., S. L. Painter, H. Viswanathan, N. Makedonska, and S. Karra 2015. "Influence of injection mode on transport properties in kilometer-scale three-dimensional discrete fracture networks". *Water Resources Research*, 51(9), 7289-7308. doi: 10.1002/2015wr017151
 40. Hyman, J. D., S. Karra, N. Makedonska, C. W. Gable, S. L. Painter, and H. S. Viswanathan 2015. "dfnWorks: A discrete fracture network framework for modeling subsurface flow and transport". *Computers & Geosciences*, 84, 10-19. doi: 10.1016/j.cageo.2015.08.001
 41. Li, Y. H. and S. Gregory 1974. "Diffusion of Ions in Sea-Water and in Deep-Sea Sediments," *Geochimica Et Cosmochimica Acta*, 38(5), 703-714.
 42. Helton, J.C., J.D. Johnson, C.J. Sallaberry, and C.B. Storlie 2006. "Survey of sampling-based methods for uncertainty and sensitivity analysis," *Reliability Engineering and System Safety*, 91(2006), 1175-1209.

ACKNOWLEDGEMENTS

The authors would like to thank Frank Perry (LANL), who gave important insights regarding potential crystalline host rock formations in the U.S., as well as members of the LANL DNFWorks Team, who helped with fracture mapping and representation of the natural system, including Hari Viswanathan (LANL), Satish Karra (LANL), Jeffrey Hyman (LANL), and Nataliia Makedonska (LANL). Ernie Hardin (SNL) provided detailed knowledge regarding repository design and thermal constraints. Sandia National Laboratories is a multi-mission laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. This paper is Sandia publication SAND2016-11750C.